AMENDMENTS TO THE CLAIMS:

Please cancel claims 12 and 14 without prejudice, and amend claims 1, 2, 6, 8-11 and

15 as set forth below.

This listing of claims will replace all prior versions and listings of claims in the

Application:

Claim 1 (currently amended): A method of aligning a query protein sequence with a

template ~~consisting of~~which comprises a set of pre-selected protein structures in a database, to

identify the structure of the template that best fits the query protein sequence, comprising the

steps of:

selecting an energy function, said energy function being a ~~sum of energy parameters~~

~~and weighting factors~~linear combination of energy parameters, with weight factors as

coefficients;

~~determining values for weighting factors in said energy function~~;

establishing linear programming (LP) constraints for threading (or aligning) said query

protein sequence with each structure in said set of pre-selected protein structures in a database;

and

performing a linear programming analysis based on a linear programming formulation

including said energy function under said constraints, to optimally align said query protein with

said template, the structure of the template that optimally aligns with the query protein

sequence being identified as the best fit.

Claim 2 (currently amended): The method of claim 1, wherein said step of determining

~~weighting~~weight factors comprises the step of using training to determine values for said

~~weighting~~weight factors.

Claim 3 (original): The method of claim 2, where said energy function comprises the function: $min \ W_m \ E_m + W_s \ E_s + W_p \ E_p + W_g \ E_g + W_{ss} \ E_{ss}$.

Claim 4 (original): The method of claim 1, where alignment gaps are confined to loops.

Claim 5 (original): The method of claim 1, where only interaction between core residues is considered.

Claim 6 (currently amended): The method of claim 1, wherein said step of performing a linear programming analysis is done on the assumption that solutions are likely to be integral.

Claim 7 (original): The method of claim 6, wherein said step of performing a linear programming analysis comprises the step of using a branch and bound technique to perform said linear programming analysis.

Claim 8 (currently amended): The method of claim 1, where said linear programming constraints ~~comprise Constraints (8) - (15).~~require that:

one core can be aligned to a unique sequence position;

conflicts between said core and the adjacent two cores are forbidden;

at most one interaction variable can have a value of 1 between any two cores that have interactions between each other;

if two cores have their alignments to the sequence respectively and also have interactions between them, then at least one interaction variable should be 1; and

the values of x (alignment variables) and y (interaction variables) are to be between 0 and 1 when the problem is relaxed to a linear program.

Claim 9 (currently amended): The method of claim 1, where said linear programming constraints ~~comprise Constraints (8), (14), (15) and (16) - (19).~~require that:

one core can be aligned to a unique sequence position;

the values of x (alignment variables) and y (interaction variables) are to be between 0

and 1 when the problem is relaxed to a linear program;

conflicts between two neighbouring cores are forbidden; and

it is guaranteed that one interaction variable has a value of 1 if and only if its two

generating x variables have a value of 1.

Claim 10 (currently amended): The method of claim 1, where said linear programming

constraints ~~comprise Constraints (8), (14), (15), (20) and (21).~~require that:

one core can be aligned to a unique sequence position;

the values of x (alignment variables) and y (interaction variables) are to be between 0

and 1 when the problem is relaxed to a linear program; and

when one x variable is 1 is equivalent to that one of the y variables generated by it is 1.

Claim 11 (currently amended): The method of claim 1, further comprising the step of

performing graph reduction to decrease the number of integer variables and speed up the LP

analysis.

Claim 12 (cancelled).

Claim 13 (original): The method of claim 1, comprising step of generating a dense contact

graph prior to said step of performing a linear programming analysis.

Claim 14 (cancelled).

Claim 15 (currently amended): A system for aligning proteins comprising:

a computer operable to align a query protein sequence with a template consisting of a

set of pre-selected protein structures in a database, to identify the structure of the template that

best fits the query protein sequence, by performing the steps of:

selecting an energy function;

determining values for ~~weighting~~weight factors in said energy function;

establishing linear programming (LP) constraints for threading (or aligning) said query protein sequence with each structure in said set of pre-selected protein structures in a database; and

performing a linear programming analysis based on a linear programming formulation including said energy function under said constraints, to optimally align said query protein with said template, the structure of the template that optimally aligns with the query protein sequence being identified as the best fit.